U.S. DEPARTMENT OF ENERGY

Argonne NATIONAL LABORATORY

Distributed Data Analysis at Scale

"Data movement, rather than computational processing, will be the constrained resource at exascale." – Dongarra et al. 2011.

Tom Peterka
tpeterka@mcs.anl.gov
http://www.mcs.anl.gov/~tpeterka
Mathematics and Computer Science Division

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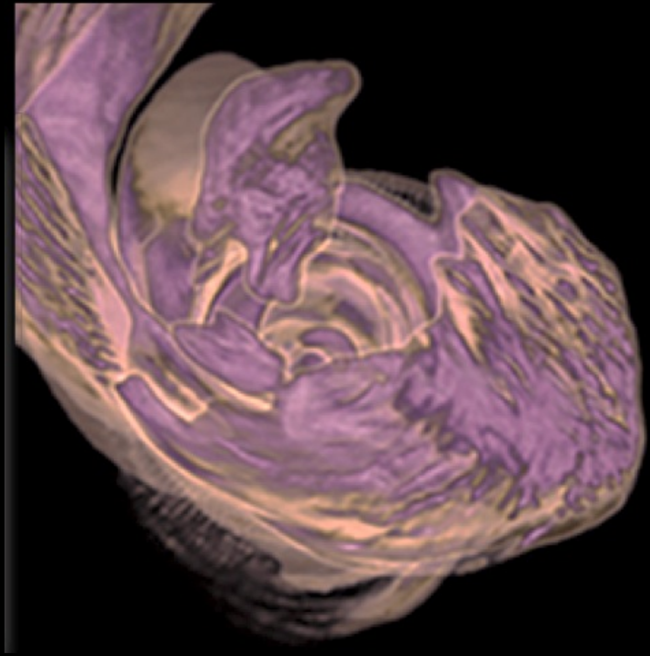
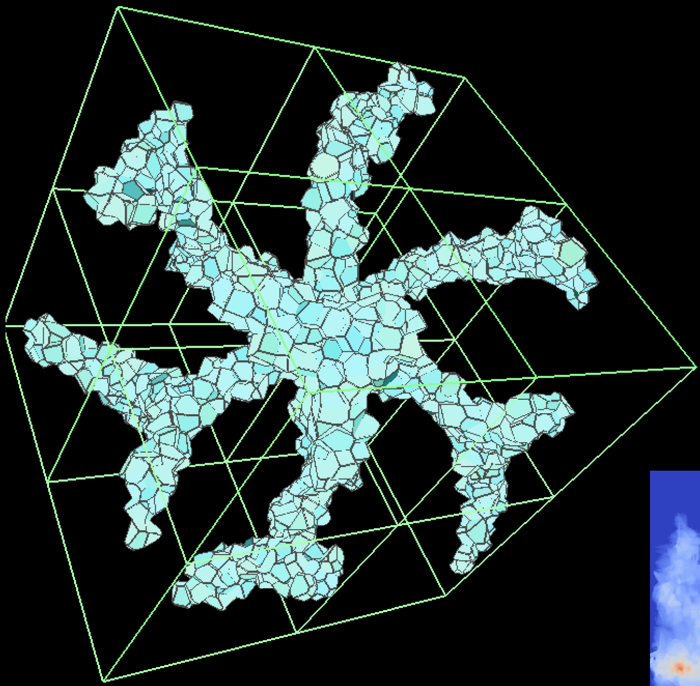
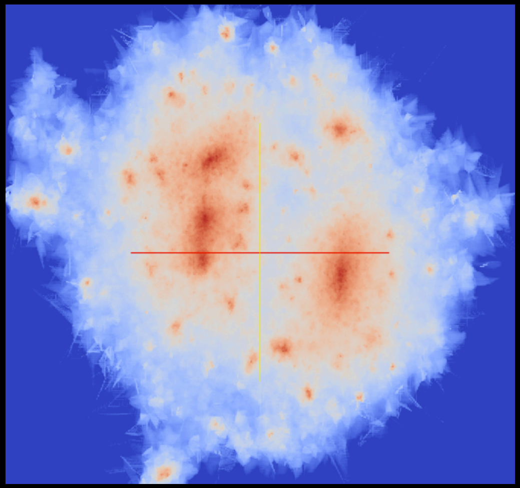
Examples



Ridge detection in meteorology



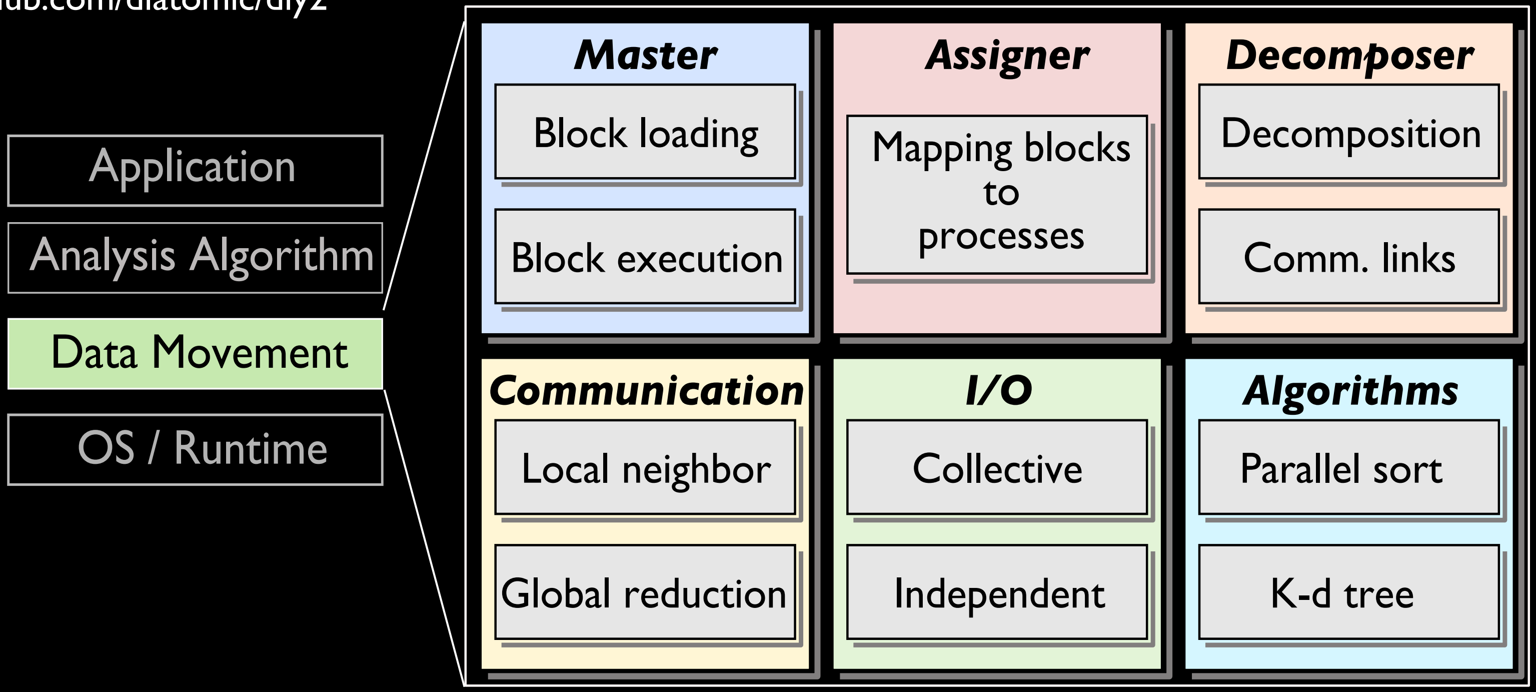
Computational geometry in molecular dynamics



Density estimation in cosmology

Common Data Movement Layer

Argonne NATIONAL LABORATORY
BERKELEY LAB
Tom Peterka Dmitriy Morozov
github.com/diatomic/diy2



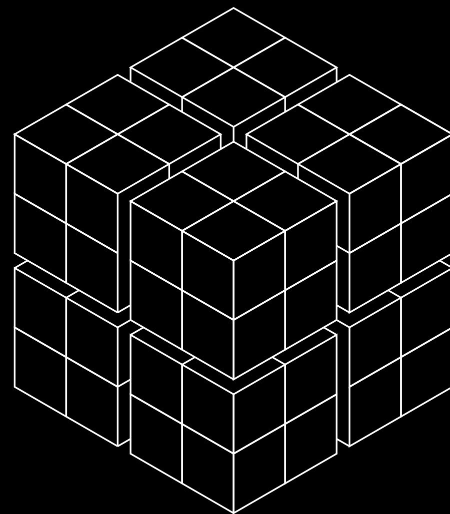
DIY is a programming model and runtime for HPC block-parallel data analytics.

- Block parallelism
- Flexible domain decomposition and assignment to resources
- Efficient reusable communication patterns
- Automatic dual in- and out-of-core execution
- Automatic block threading

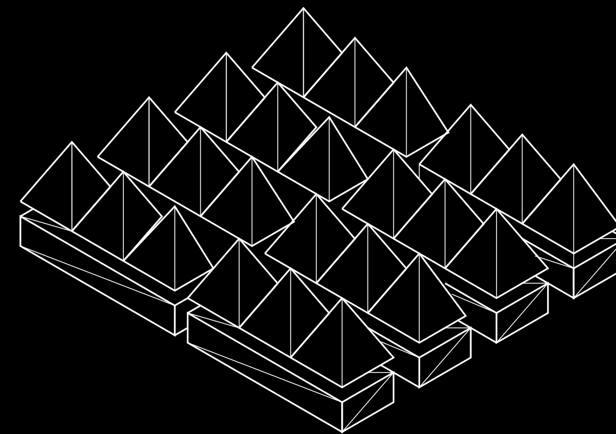
Basic Concepts

Partition Data Into Blocks

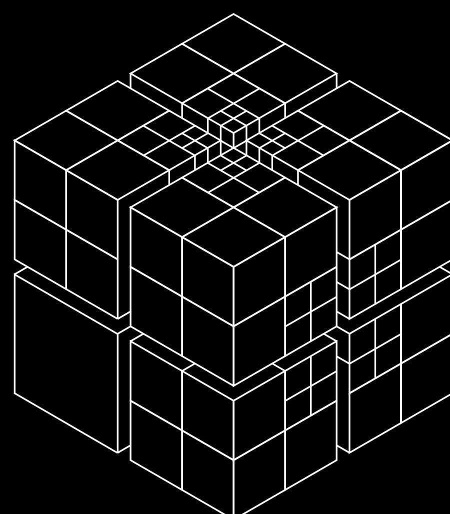
The block is the basic unit of data decomposition. Original dataset is decomposed into generic subsets called blocks, and associated analysis items live in the same blocks. Blocks don't have to be "blocky." Any subdivision of data (eg., a set of graph nodes, a group of particles, etc.) is a block.



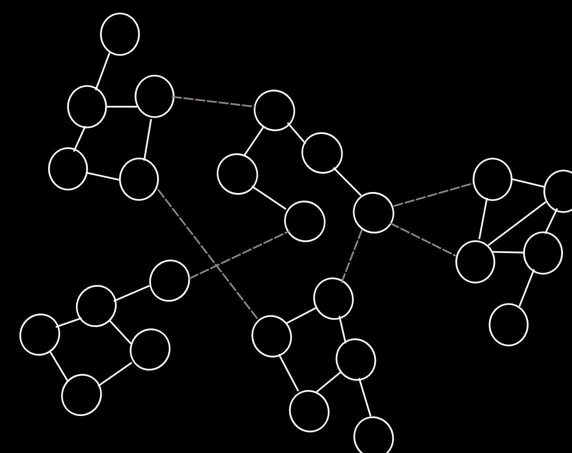
Structured Grid



Unstructured Mesh



AMR Grid



Graph

Multiple Regular Decompositions

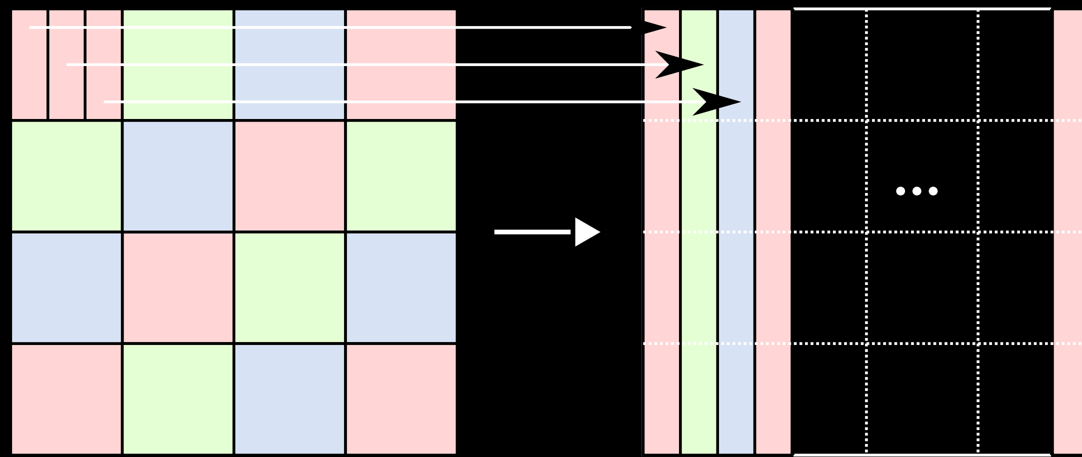
1. Decomposition can be a regular grid of blocks or a k-d tree.

2. For a regular grid, constraints on numbers of blocks can be imposed to get pencil or slab shapes.

3. Multiple decompositions can co-exist.

Original block decomposition

Slab or pencil decomposition for FFT

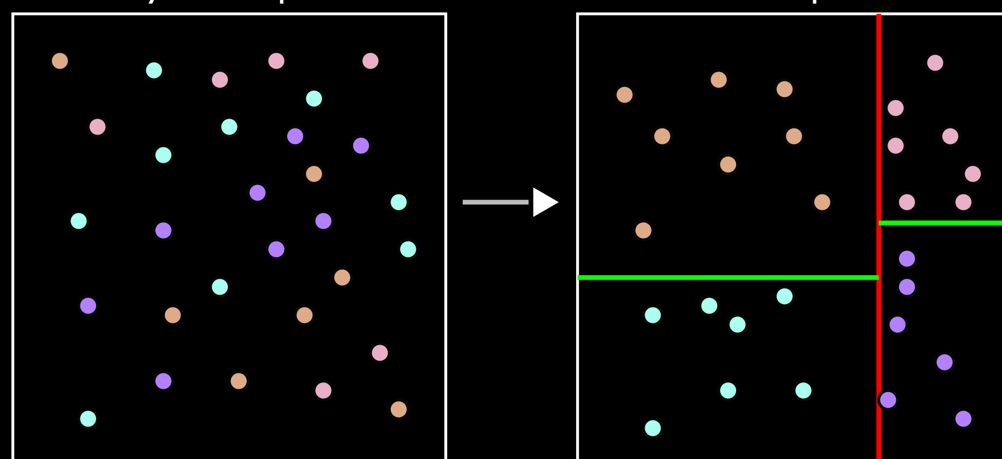


16 blocks, 3 procs indicated by color

Need not be same number of blocks

Original data
Arbitrary decomposition

Kd-tree decomposition

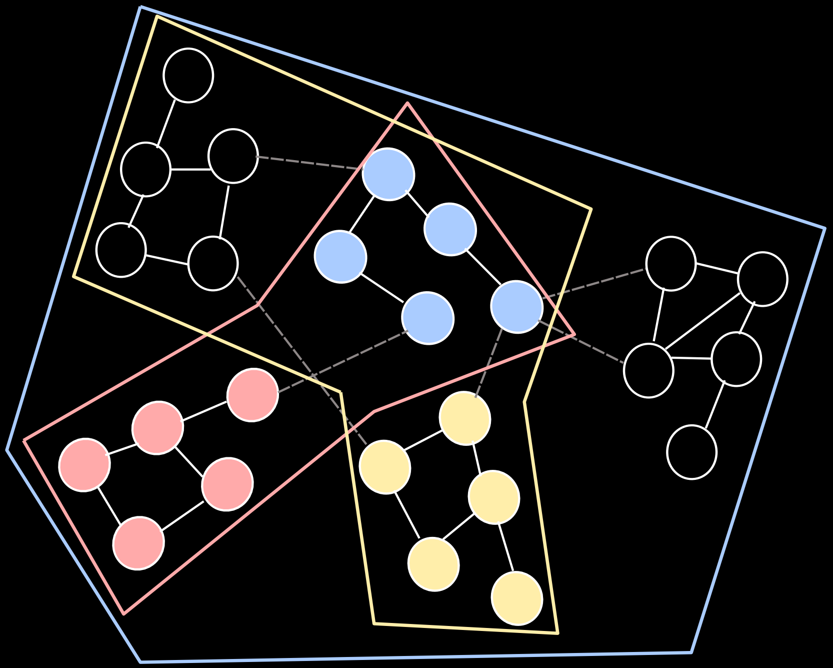


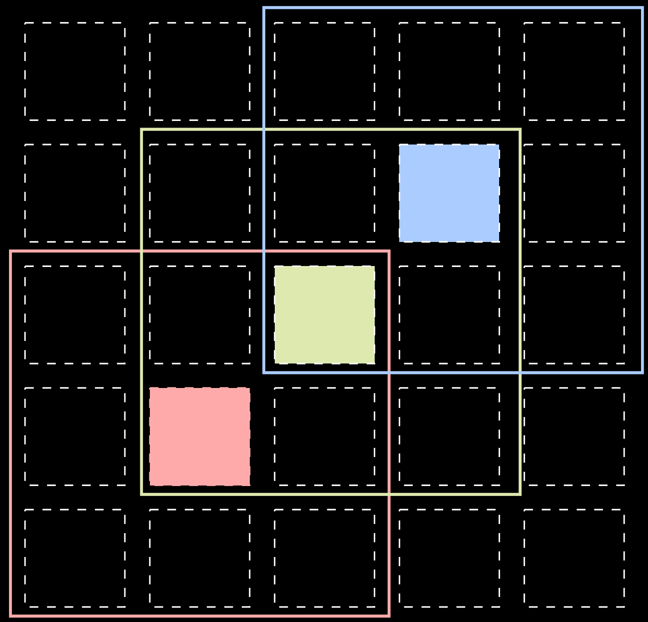
4 blocks indicated by color.
No spatial locality assumed.

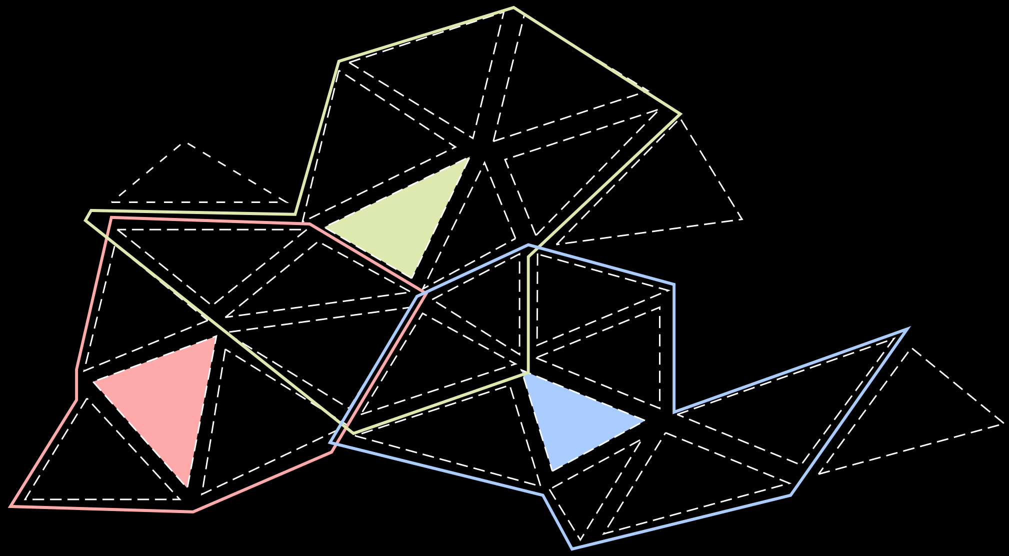
4 new blocks spatially contiguous and load balanced by number of objects in each.

Neighborhood Links

- Limited-range communication
- Allow arbitrary groupings
- Distributed, local data structure and knowledge of other blocks (not master-slave global knowledge)







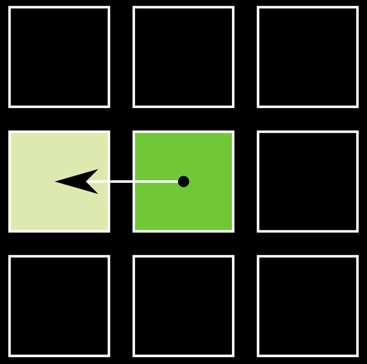
Examples of 3 neighborhoods in a regular grid, unstructured mesh, and graph.

Communicate over the Link

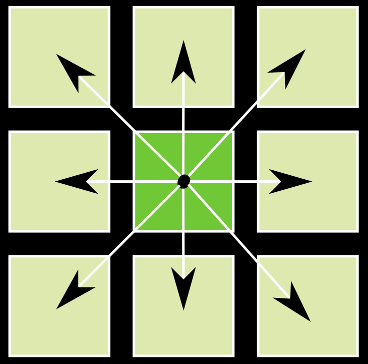
DIY provides point to point and different varieties of collectives within a neighborhood via its enqueue/exchange/dequeue mechanism.

How to enqueue items for neighbor exchange

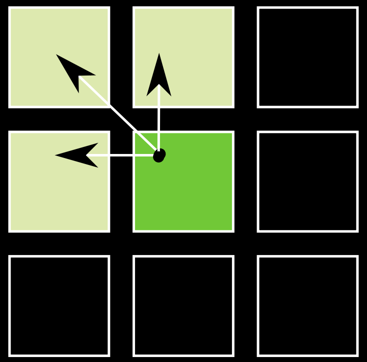
- DIY offers several options
- Send to a particular neighbor or neighbors, send to all nearby neighbors, send to all neighbors
- Support for periodic boundary conditions



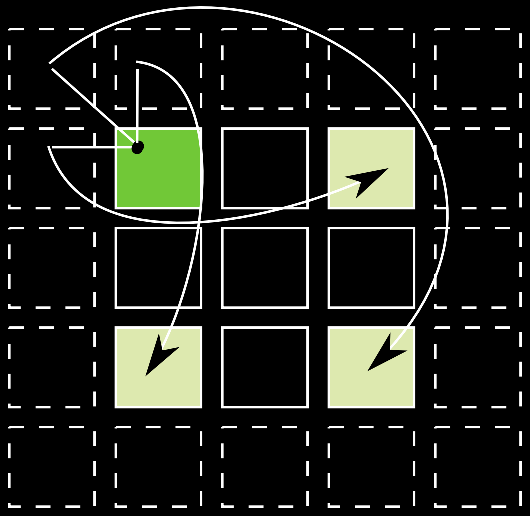
Send to only specific neighbors, indicated in various ways



Send to all neighbors



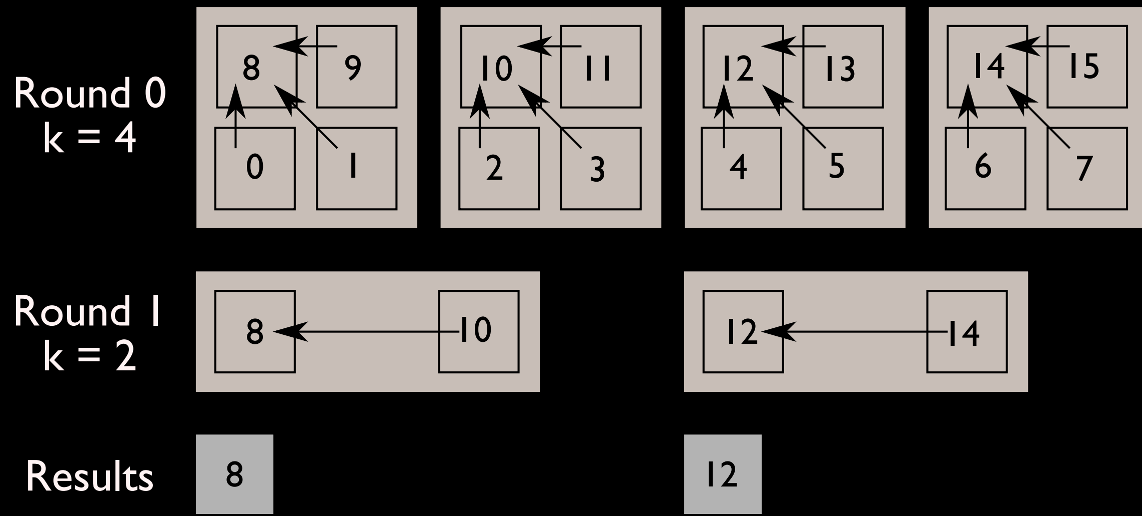
Send to all neighbors near enough to a target point



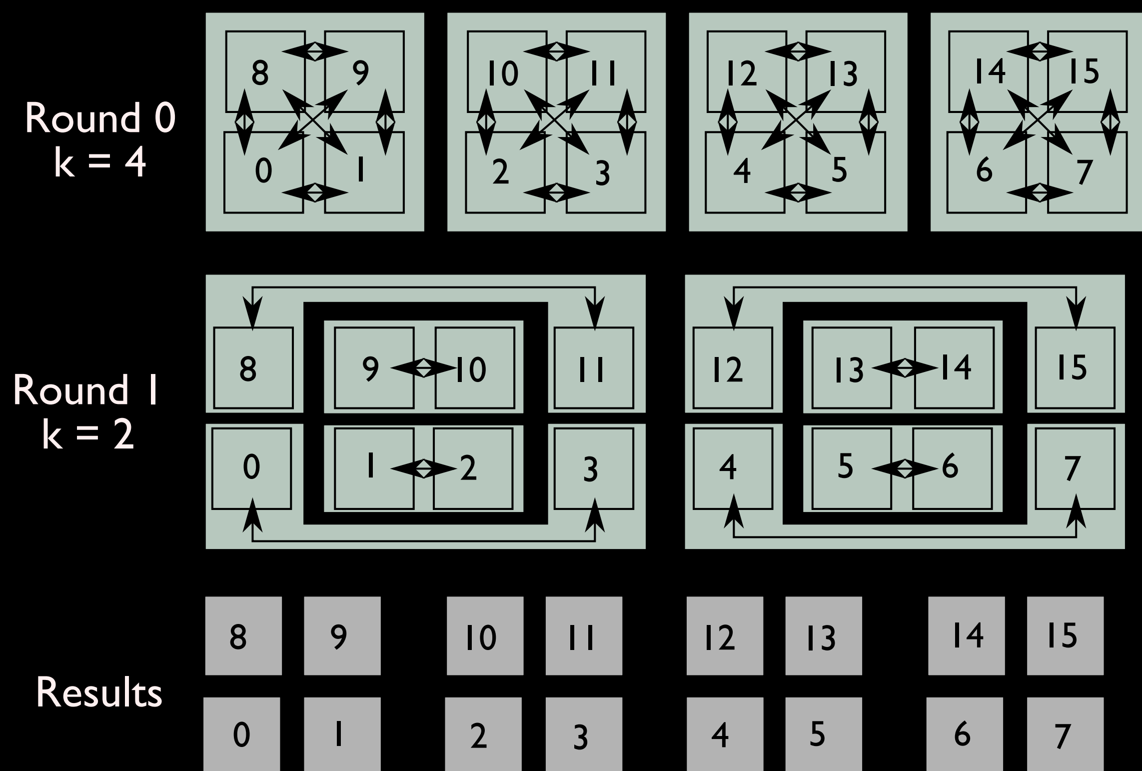
Support for wraparound neighbors (periodic boundary conditions)

Global Communication Patterns

Merge-reduce



Swap-reduce



Example Usage

```
// initialization
Master                  master(world, num_threads, mem_blocks, ...);
ContiguousAssigner      assigner(world.size(), tot_blocks);
decompose(dim, world.rank(), domain, assigner, master);

// compute, neighbor exchange
master.foreach(&foo);
master.exchange();

// reduction
RegularSwapPartners(dim, tot_blocks, k);
reduce(master, assigner, partners, &foo);

// callback function for each block
void foo(void* b, const Proxy& cp, void* aux)
{
    for (size_t i = 0; i < in.size(); i++)
        cp.dequeue(cp.link()->target(i), incoming_data);
    // do work on incoming data
    for (size_t i = 0; i < out.size(); i++)
        cp.enqueue(cp.link()->target(i), outgoing_data[i]);
}
```

One Example in Detail

Self-Adaptive Density Estimation

Sampling a regular density field from a distribution of particle positions using a Voronoi tessellation as an intermediate data model.

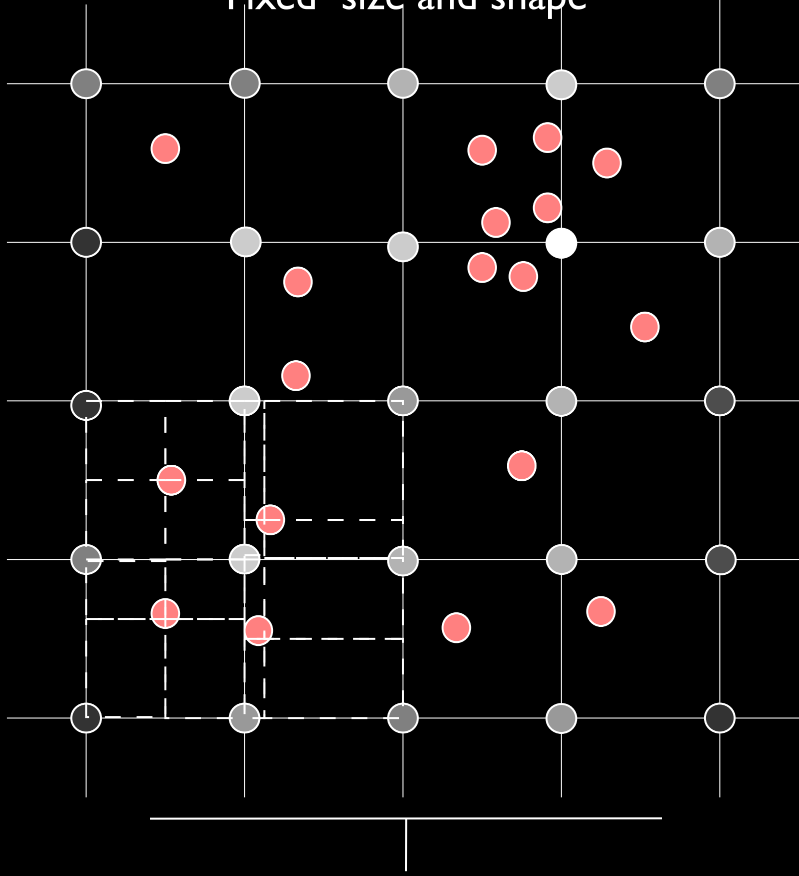
Key Ideas

- Convert discrete particle data into continuous function that can be interpolated, differentiated, interpolated, represented as a regular grid (field)
- Automatically adaptive window size and shape
- Comparison with CIC using synthetic and actual data
- Voronoi tessellation and density estimation computed in parallel on distributed-memory HPC machines

Estimation Kernels

CIC

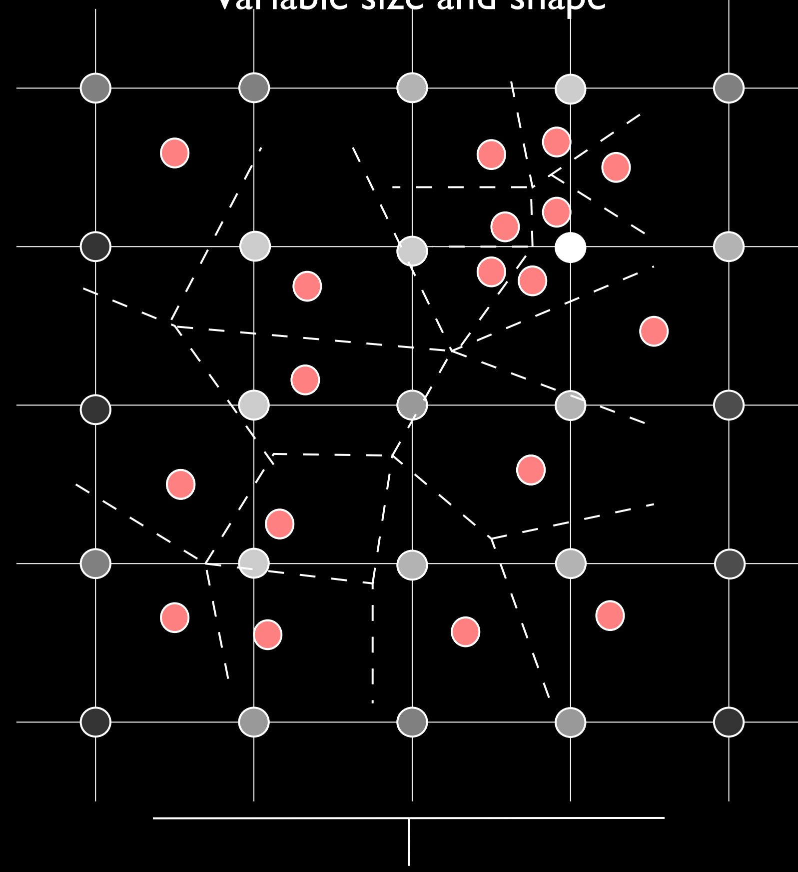
Fixed size and shape



In cloud-in-cell (CIC) methods, particles are distributed to a fixed number of grid points.

TESS

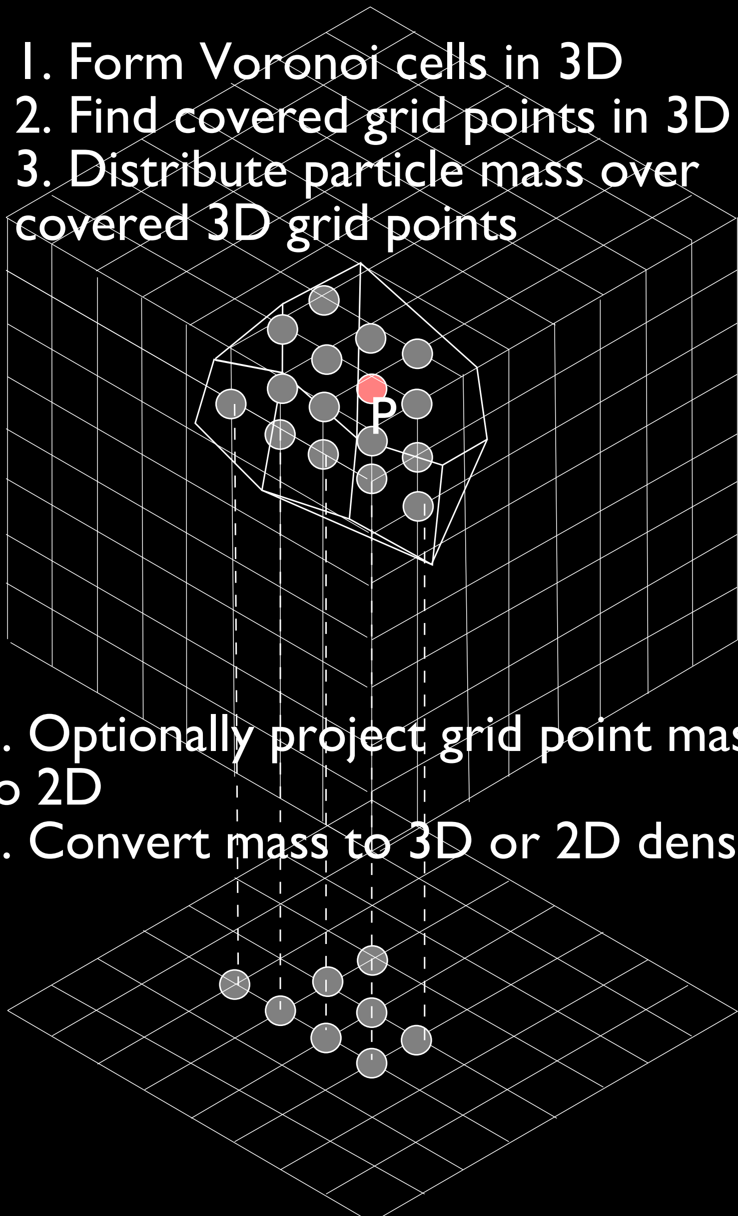
Variable size and shape



In tessellation (TESS) methods, particles are distributed to a variable number of grid points according to the Voronoi or Delaunay tessellation that has variable size and shape cells.

Overall Algorithm

1. Form Voronoi cells in 3D
2. Find covered grid points in 3D
3. Distribute particle mass over covered 3D grid points
4. Optionally project grid point mass to 2D
5. Convert mass to 3D or 2D density




```
for (all Voronoi cells) {

  compute grid points in Voronoi cell interior

  for (all interior grid points) {

    if (grid point is inside local block)
      add mass contribution to grid point

    else
      send mass contribution to neighbor block
         containing grid point and add it there

    if (2D projection) {
      accumulate mass at 2D pixel
      divide by pixel area for 2D density
    }

    else
       divide by voxel volume for 3D density

  } // interior grid points

} // Voronoi cells
```

Accuracy

Navarro-Frenk-White (NFW)

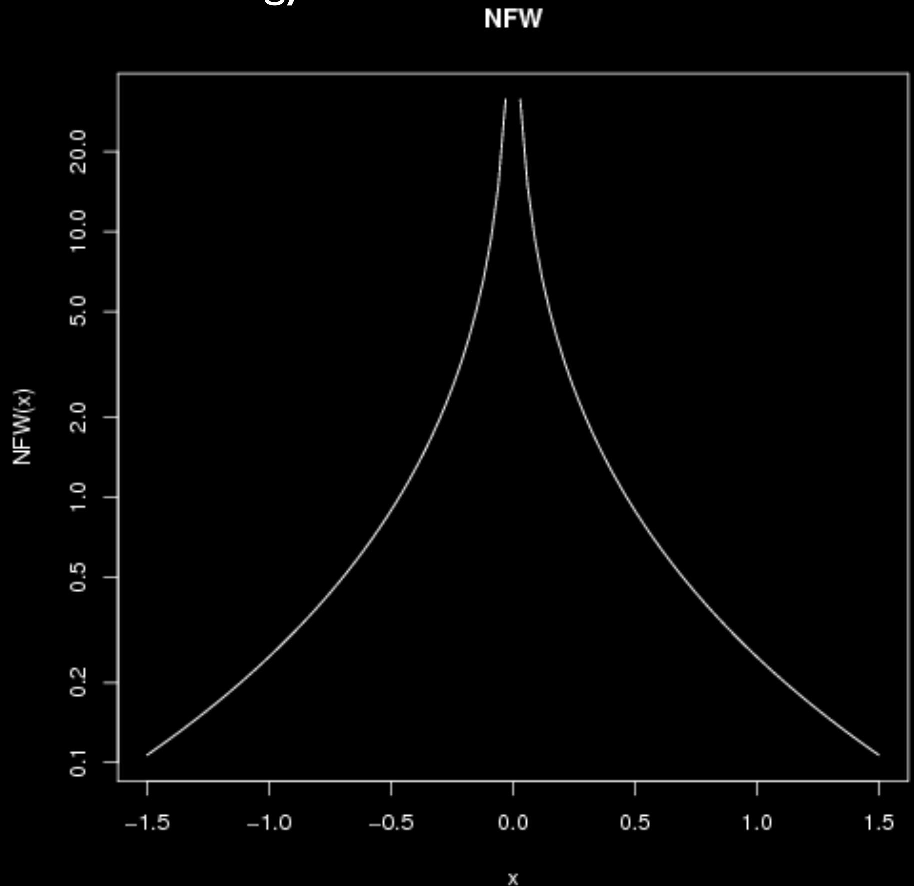
Synthetic dataset derived from an analytical density function commonly used in cosmology.

k is a constant, 1 for us

$\rho\,(r)$ is Monte Carlo sampled to get test set of particles

Ground truth is 2D plot of $\rho\,(r)$

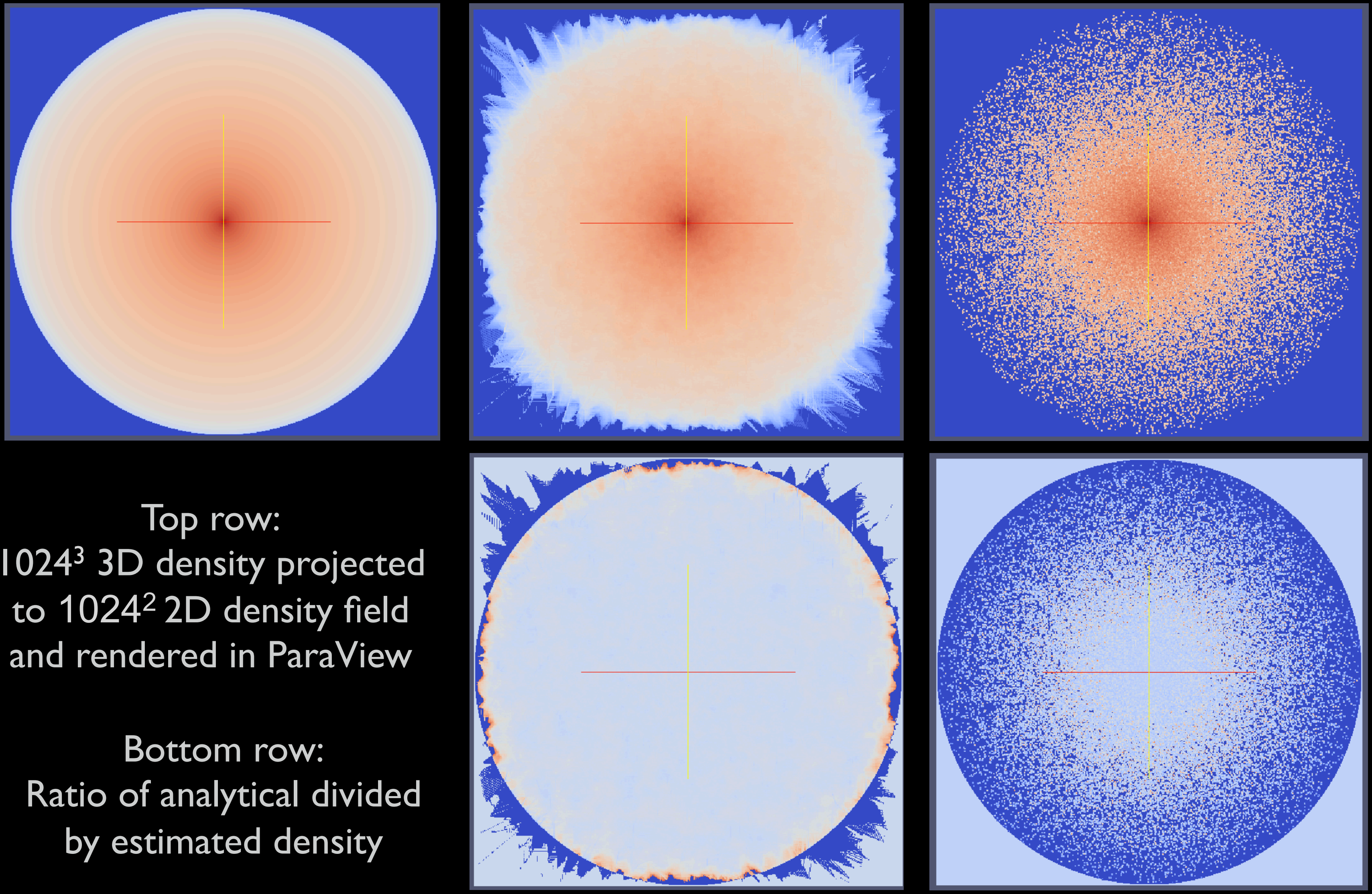
We limit r to [-1.5, 1.5] and NFW(r) to 10^6



$$\rho(r) = \frac{k}{(r(r+1)^2)}$$

NFW 2D Density Fields

Analytical | TESS | CIC

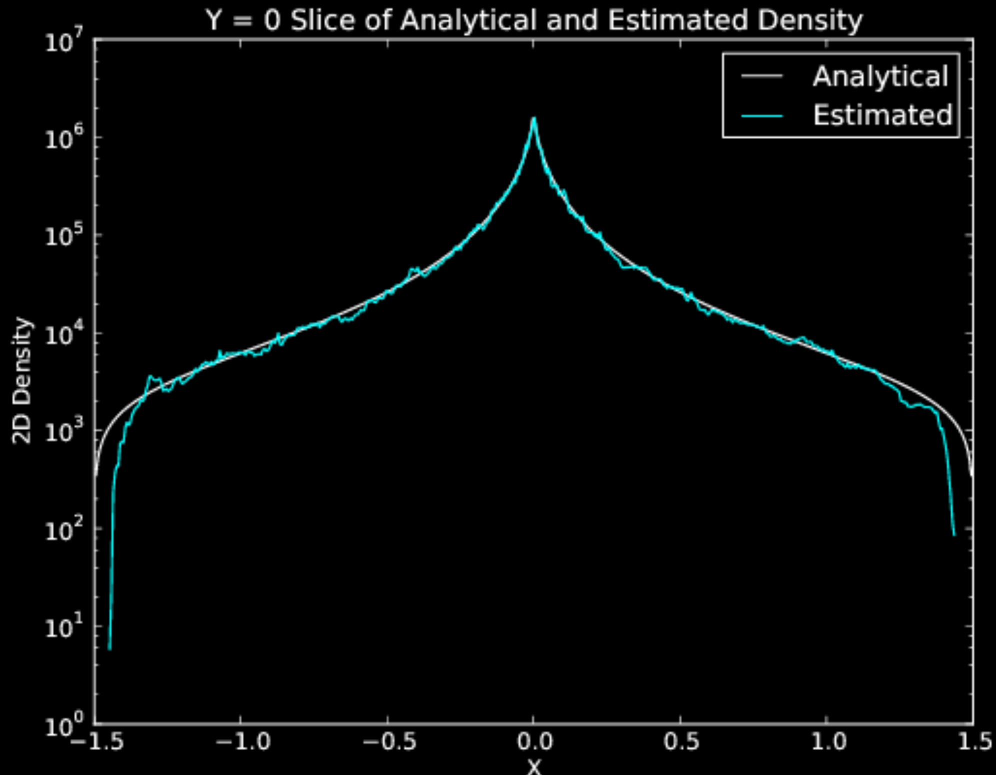


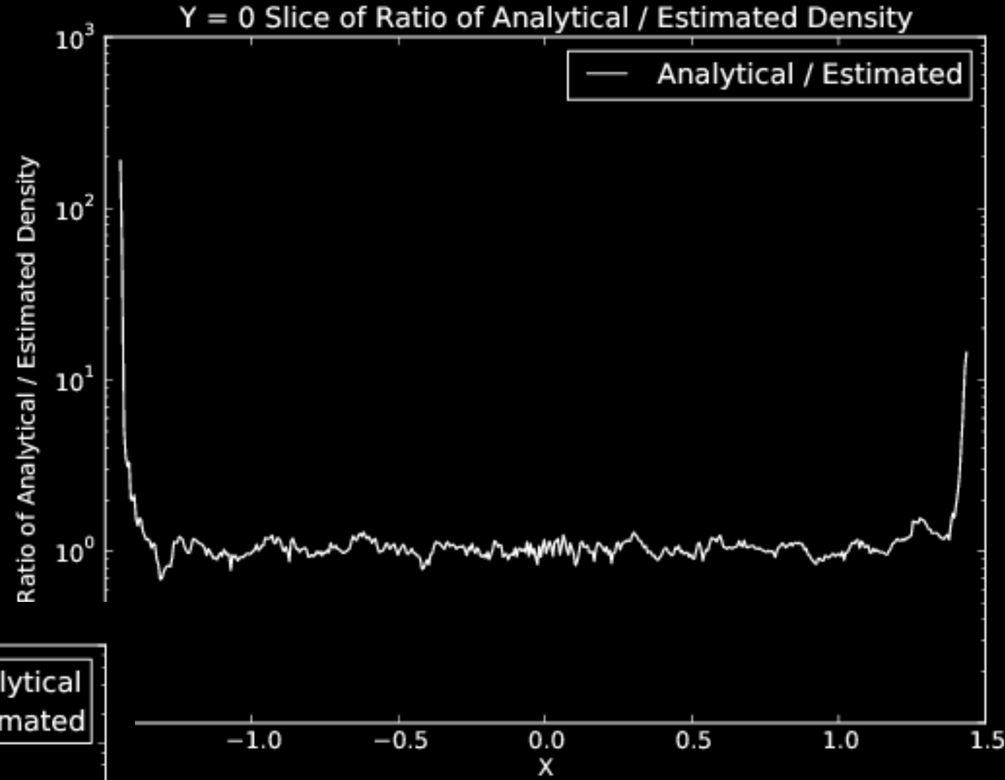
Top row:
1024^3 3D density projected to 1024^2 2D density field and rendered in ParaView

Bottom row:
Ratio of analytical divided by estimated density

TESS

Comparison between analytical 2D density and estimated density at $y = 0$ cross section

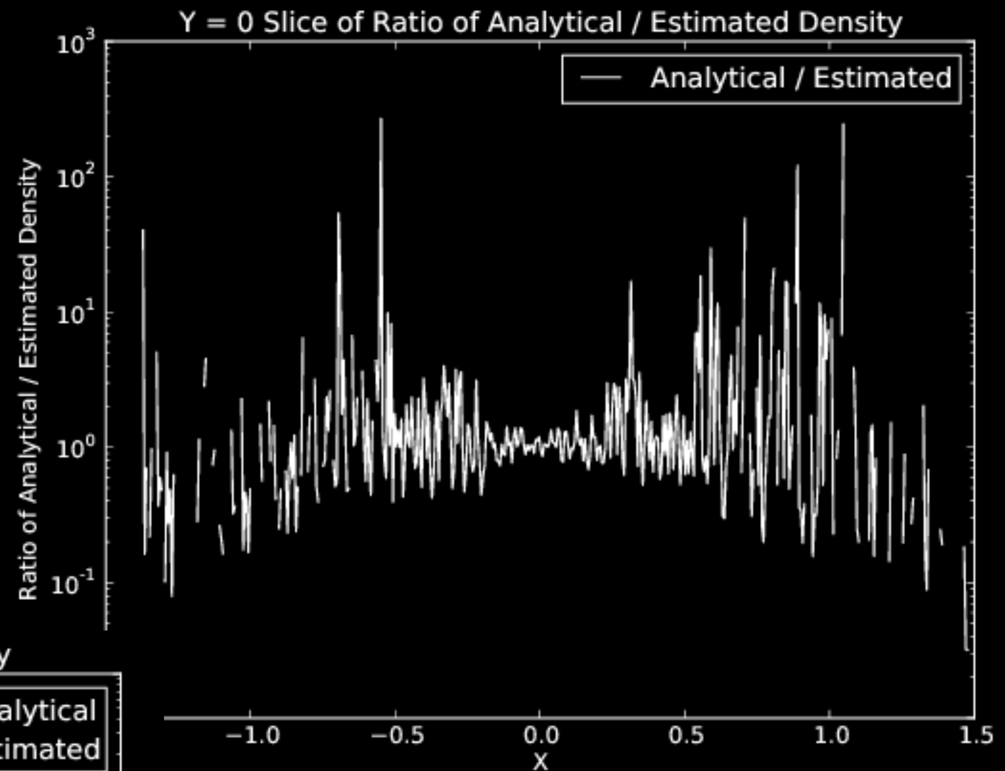


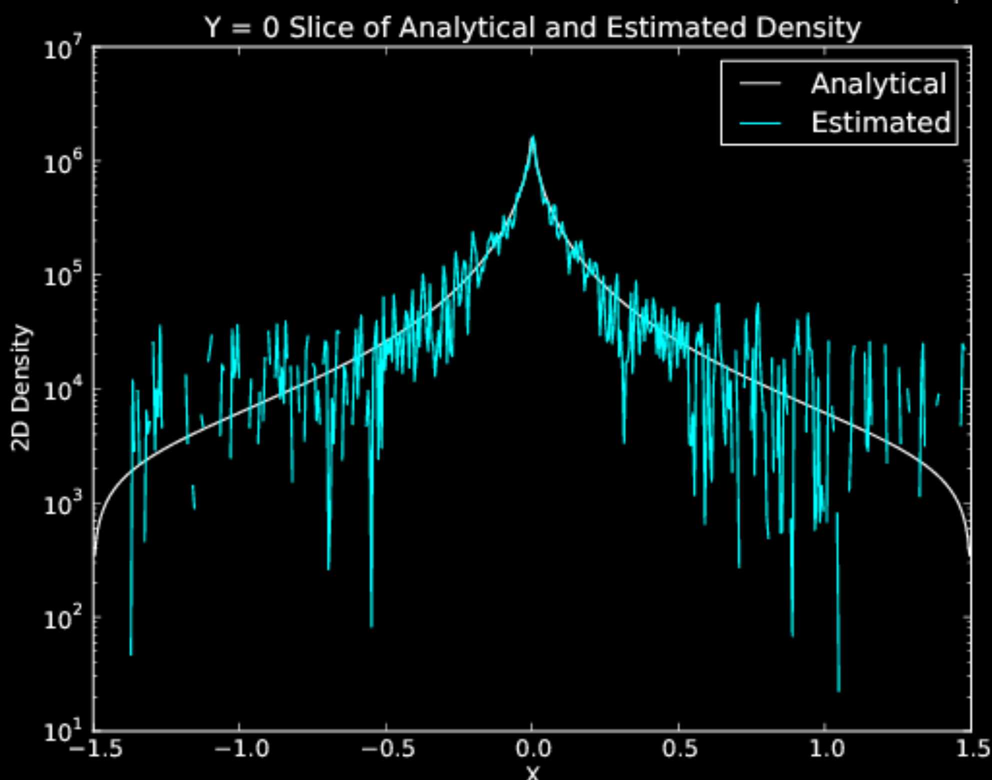


Ratio between analytical 2D density divided by estimated density at $y = 0$ cross section

CIC

Comparison between analytical 2D density and estimated density at $y = 0$ cross section

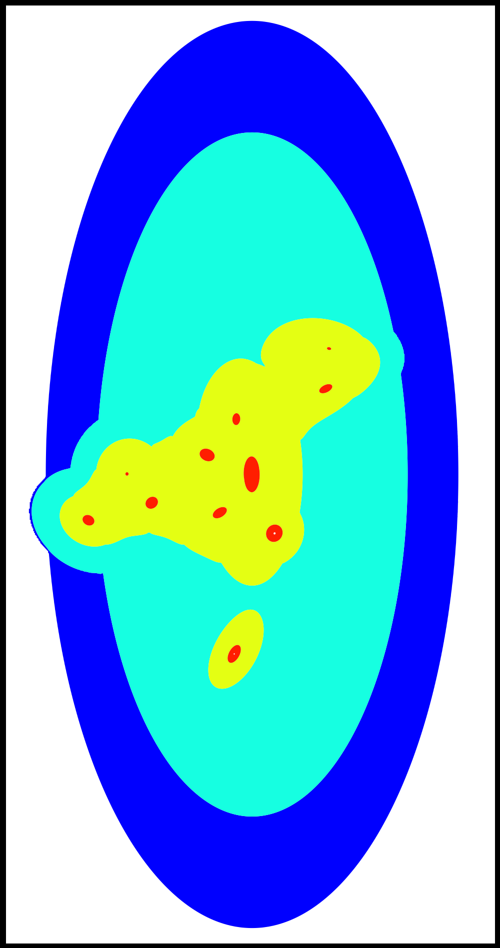




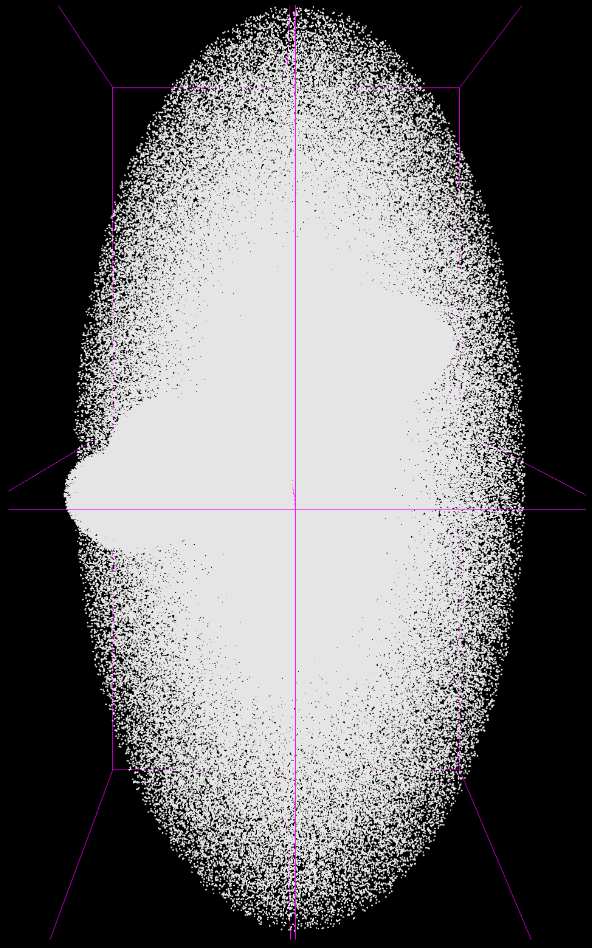
Ratio between analytical 2D density divided by estimated density at $y = 0$ cross section

Complex NFW (CNFW)

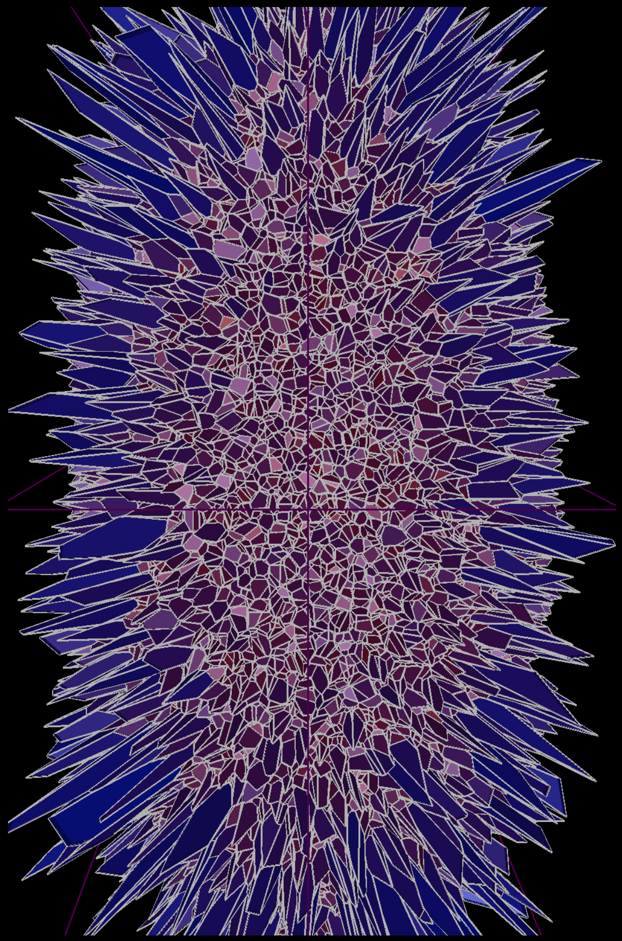
Our second synthetic dataset is a combination of several NFWs of varying cutoff densities and asymmetric scaling factors.



Analytical cutoff density contours

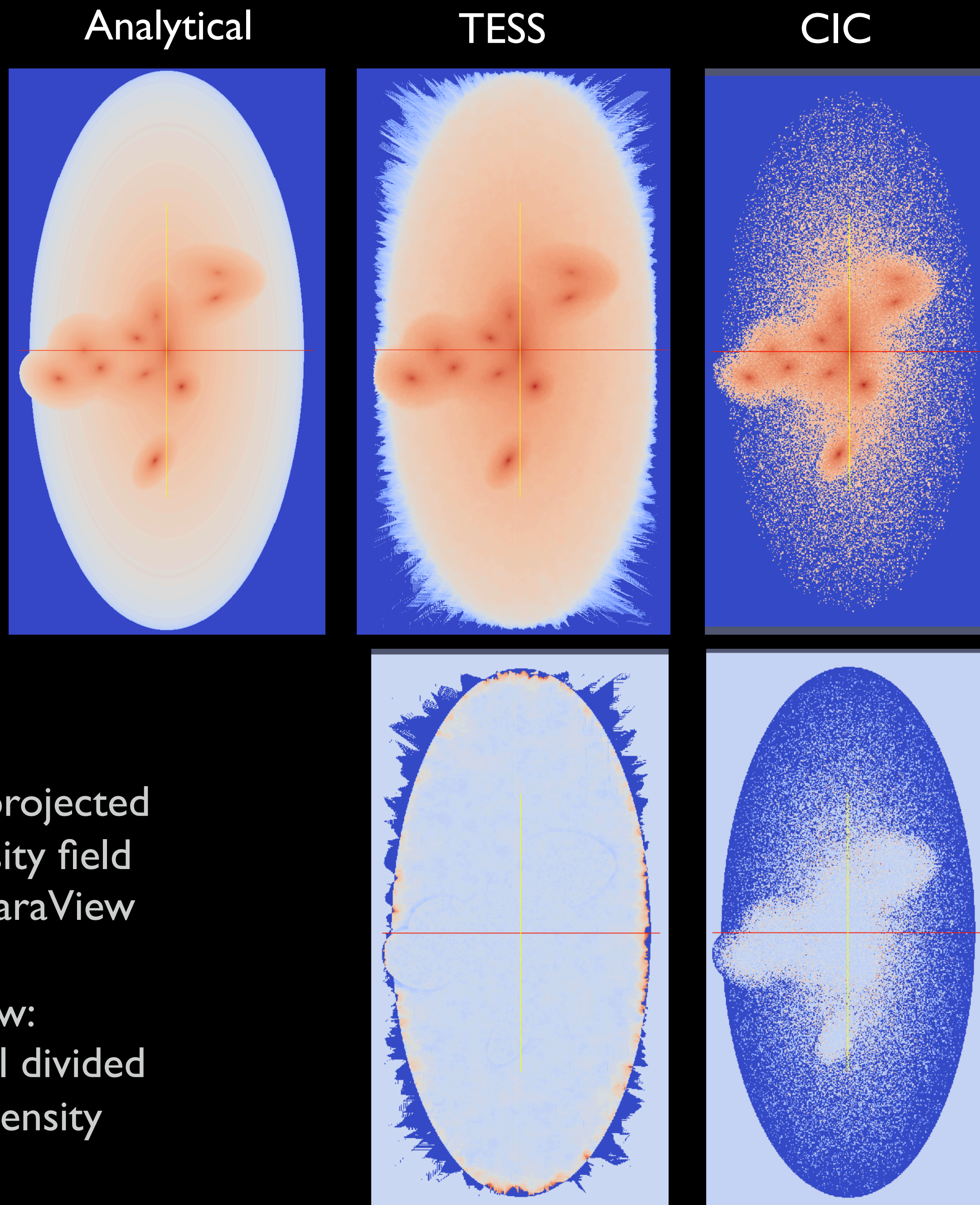


2e5 sampled particles



Voronoi tessellation

CNFW 2D Density Fields



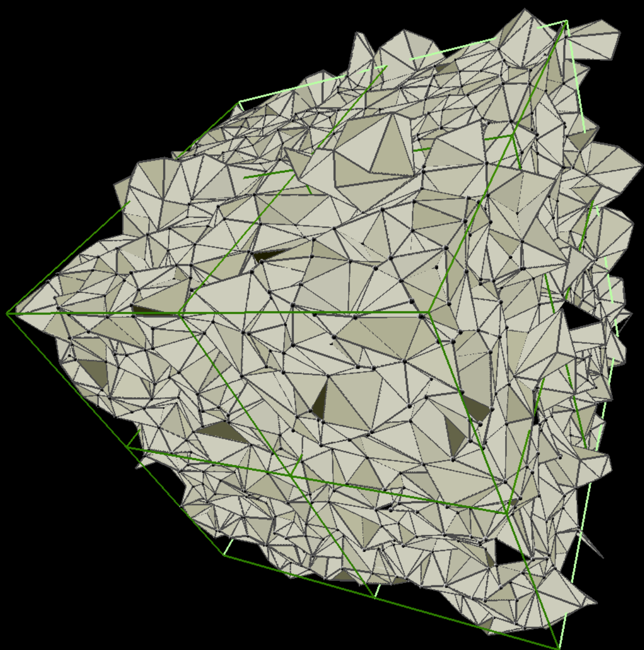
Top row:
1024^3 3D density projected
to 1024^2 2D density field
and rendered in ParaView

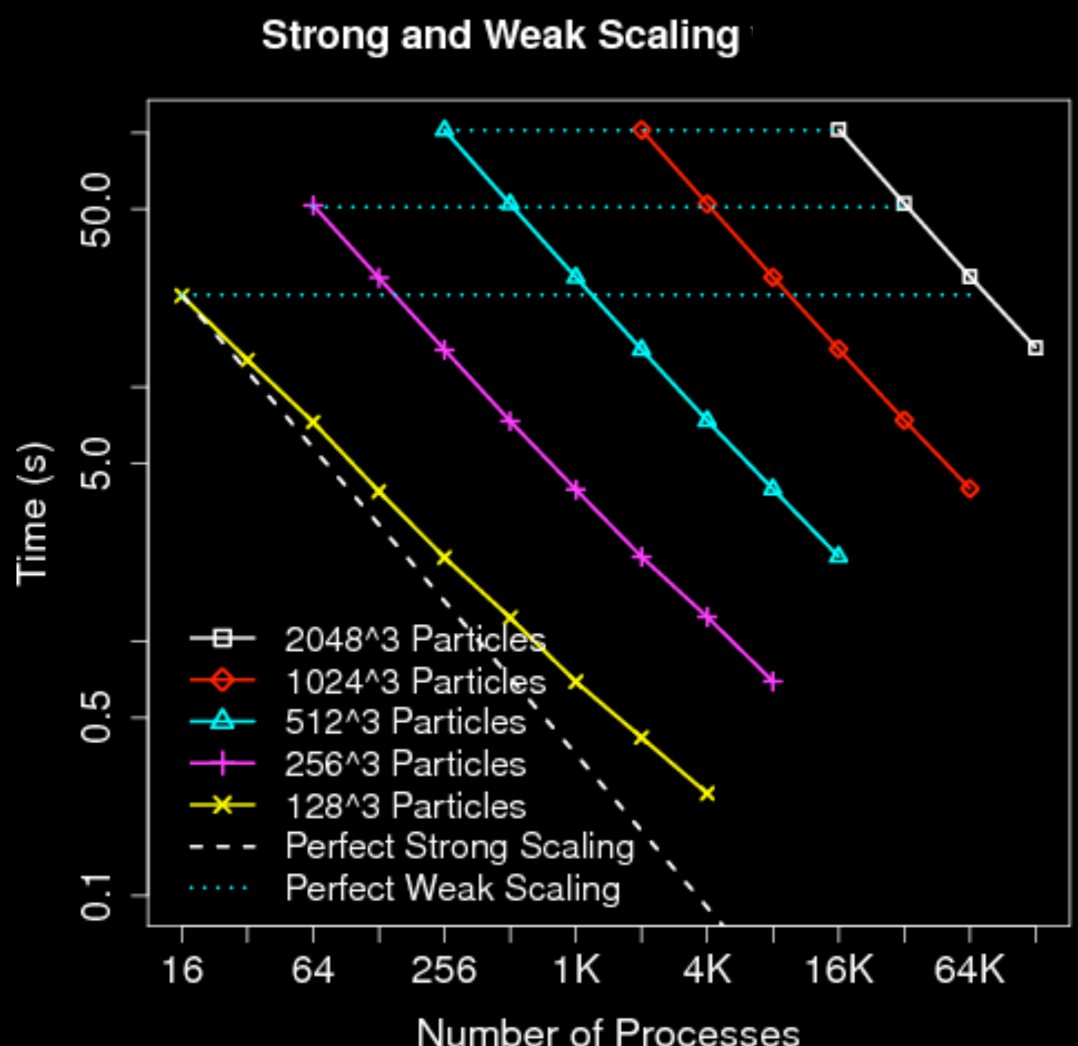
Bottom row:
Ratio of analytical divided
by estimated density

With Dmitriy Morozov and Carolyn Phillips

[github.com/diatomic/tess2]

Performance of Voronoi Tessellation





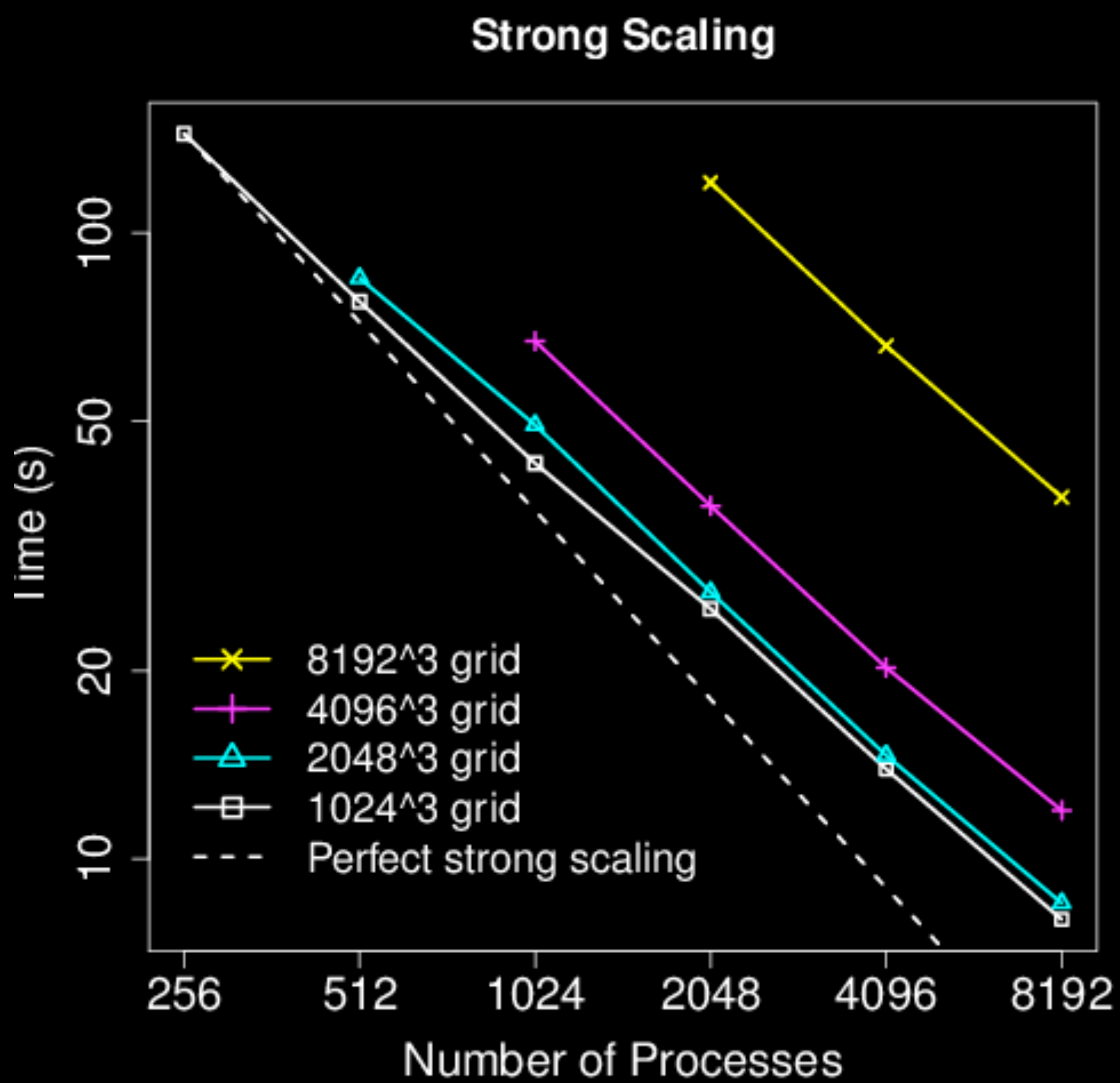
Strong and weak scaling for up to 2048^3 synthetic particles and up to 128K processes (excluding I/O) shows up to 90% strong scaling and up to 98% weak scaling.

Peterka et al., High-Performance Computation of Distributed-Memory Parallel 3D Voronoi and Delaunay Tessellation. SC14.

With Hadrien Croubois, Nan Li, Steve Rangel, and Franck Cappello

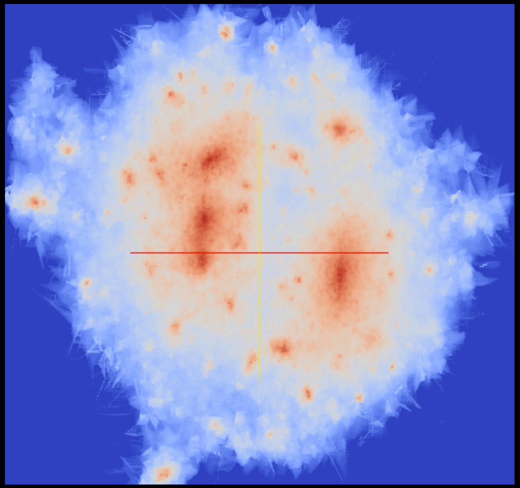
[github.com/diatomic/tess2]

Performance of Density Estimation



Left: Strong scaling of estimating the density of 512^3 synthetic particles onto grids of various sizes.

Below: Density estimation of one halo of dark matter particles in a cosmology simulation



Peterka et al., Self-Adaptive Density Estimation, SIAM SISC 2016.

Recap

How to DIY Data Analysis

DIY data movement library for parallelizing data analysis

- Decompose data into blocks
- Assign blocks to processing elements
- Have several decompositions at once
- Overload blocks, migrate blocks between processing elements
- Communicate between blocks
- Migrate blocks in and out of core
- Thread blocks with finer-grained processing elements

Tessellation-based density estimation example

- Parameter-free
- Shape-free
- Automatically adaptive
- Higher quality estimation in high-contrast data
- Scalable parallel performance

References

DIY Papers

- Peterka, Ross, Kendall, Gyulassy, Pascucci, Shen, Lee, Chaudhuri: Scalable Parallel Building Blocks for Custom Data Analysis. LDAV 2011.
- Peterka, Ross: Versatile Communication Algorithms for Data Analysis. EuroMPI 2012.
- Morozov, Peterka: Block-Parallel Data Analysis with DIY2. Submitted to LDAV 2016.

Selected DIY Application Papers

- Morozov, Peterka: Efficient Delaunay Tessellation through K-D Tree Decomposition. To appear SC16.
- Peterka, Croubois, Li, Rangel, Cappello: Self-Adaptive Density Estimation of Particle Data. SIAM Journal on Scientific Computing SISC Special Section on CSE 2015.
- Peterka, Morozov, Phillips: High-Performance Computation of Distributed-Memory Parallel 3D Voronoi and Delaunay Tessellation. SC14.
- Lu, Shen, Peterka: Scalable Computation of Stream Surfaces on Large Scale Vector Fields. SC14.
- Nashed, Vine, Peterka, Deng, Ross, Jacobsen: Parallel Ptychographic Reconstruction. Optics Express 2014.
- Gyulassy, Peterka, Pascucci, Ross: The Parallel Computation of Morse-Smale Complexes. IPDPS 2012.
- Nouanesengsy, Lee, Lu, Shen, Peterka: Parallel Particle Advection and FTLE Computation for Time-Varying Flow Fields. SC12.
- Chaudhuri, A., Lee-T.-Y., Zhou, B., Wang, C., Xu, T., Shen, H.-W., Peterka, T., Chiang, Y.-J.: Scalable Computation of Distributions from Large Scale Data Sets. LDAV 2012.

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People
Dmitriy Morozov (LBNL)

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Tom Peterka
tpeterka@mcs.anl.gov
http://www.mcs.anl.gov/~tpeterka
Mathematics and Computer Science Division